

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S1	2	("5925636").PN.	USPAT; DERWENT	OR	OFF	2006/12/11 11:14
S2	352	((549/303) or (548/364.4)).CCLS.	USPAT; DERWENT	OR	OFF	2006/12/11 11:15

11/12/2006,10525685c.trn

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* * * * * Welcome to STN International * * * * *

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NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive
NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced
NEWS 5 AUG 30 CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6 SEP 11 CA/CAplus enhanced with more pre-1907 records
NEWS 7 SEP 21 CA/CAplus fields enhanced with simultaneous left and right
truncation
NEWS 8 SEP 25 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new
classification scheme
NEWS 12 OCT 19 LOGOFF HOLD duration extended to 120 minutes
NEWS 13 OCT 19 E-mail format enhanced
NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available
NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in
multiple databases
NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN
has been enhanced and reloaded
NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field
NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality
NEWS 19 NOV 10 CA/CAplus F-Term thesaurus enhanced
NEWS 20 NOV 10 STN Express with Discover! free maintenance release Version
8.01c now available
NEWS 21 NOV 13 CA/CAplus pre-1967 chemical substance index entries enhanced
with preparation role
NEWS 22 NOV 20 CAS Registry Number crossover limit increased to 300,000 in
additional databases
NEWS 23 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased
to 50,000
NEWS 24 NOV 20 CA/CAplus patent kind codes will be updated
NEWS 25 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 26 DEC 11 CAS REGISTRY chemical nomenclature enhanced

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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NEWS X25 X.25 communication option no longer available

11/12/2006,10525685c.trn

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:44:16 ON 11 DEC 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:44:26 ON 11 DEC 2006

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STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

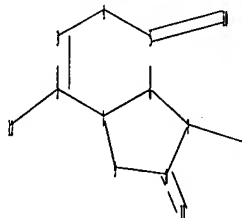
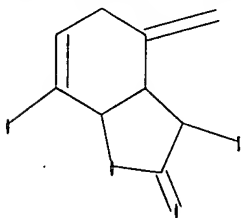
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10525685c.str



chain nodes :

10 11 12 13

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

11/12/2006,10525685c.trn

2-12 5-10 7-13 8-11

ring bonds :

1-2 1-6 1-9 2-3 3-4 4-5 5-6 6-7 7-8 8-9

exact/norm bonds :

1-2 1-6 1-9 2-3 2-12 3-4 4-5 5-6 6-7 7-8 7-13 8-9 8-11

exact bonds :

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Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

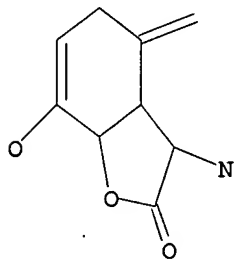
11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:45:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 80 TO ITERATE

100.0% PROCESSED 80 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1064 TO 2136

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 10:45:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1456 TO ITERATE

100.0% PROCESSED 1456 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> file hcaplus

11/12/2006,10525685c.trn

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	167.15

FILE 'HCAPLUS' ENTERED AT 10:45:12 ON 11 DEC 2006
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FILE COVERS 1907 - 11 Dec 2006 VOL 145 ISS 25
FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 4 L3

=> d ed abs ibib hitstr 1-4

L4 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 ED Entered STN: 11 Aug 2005

AB The invention relates to an improved method for cultivating the fungus *Penicillium chrysogenum*, especially strain KIP 3201, for producing the antitumoral natural substance Sorbicillactone A and its derivative in an optimized manner and in large amounts. The invention also relates to an optimized method for obtaining and purifying said substance from the fungal biomass and from the culture medium. The invention also describes the biol. activity of Sorbicillactone A and investigations relating to the

genotoxicity of the compound
 ACCESSION NUMBER: 2005:729517 HCAPLUS
 DOCUMENT NUMBER: 143:171404
 TITLE: Production and purification of sorbicillactone A
 INVENTOR(S): Bringmann, Gerhard; Lang, Gerhard; Gulder, Tobias; Schaumann, Karsten; Mueller, Werner E. G.; Perovic-Ottstadt, Sanja; Stoehr, Ruediger; Wiese, Jutta; Schmaljohann, Rolf; Imhoff, Johann
 PATENT ASSIGNEE(S): Johannes Gutenberg-Universitaet Mainz, Germany; Julius-Maximilians-Universitaet Wuerzburg
 SOURCE: PCT Int. Appl., 36 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

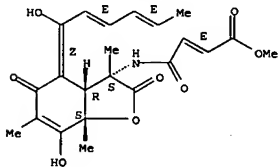
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005072711	A2	20050811	WO 2005-EP923	20050131
WO 2005072711	A3	20050915		
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PRIORITY APPLN. INFO.:
 IT 664987-12-6P, Sorbicillactone A
 RL: BMF (Bioindustrial manufacture); BSU (Biological study, unclassified);
 CPS (Chemical process); PEP (Physical, engineering or chemical process);

L4 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 ED Entered STN: 11 Aug 2005
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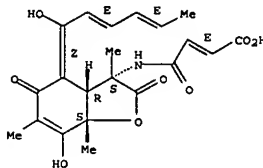
AB The invention relates to an improved method for cultivating the fungus *Penicillium chrysogenum*, especially strain KIP 3201, for producing the antitumoral natural substance Sorbicillactone A and its derivative in an optimized manner and in large amounts. The invention also relates to an optimized method for obtaining and purifying said substance from the fungal biomass and from the culture medium. The invention also describes the biol. activity of Sorbicillactone A and investigations relating to the

genotoxicity of the compound
 Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



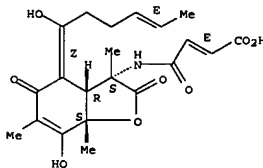
L4 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 ED Entered STN: 11 Aug 2005
 GI

Absolute stereochemistry.
 Double bond geometry as shown.



IT 861434-14-2P, DihydroSorbicillactone A
 RL: BMF (Bioindustrial manufacture); BSU (Biological study, unclassified);
 PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
 (production and purification of sorbicillactone A)
 RN 861434-14-2 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[[4E]-1-hydroxy-4-hexenylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuran-2-yl]amino]-4-oxo-, (2E)- (9CI) (CA INDEX NAME)]

Absolute stereochemistry.
 Double bond geometry as shown.



IT 861434-12-0P, Sorbicillactone A methyl ester
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP

L4 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN
 ED Entered STN: 24 Jun 2005
 GI

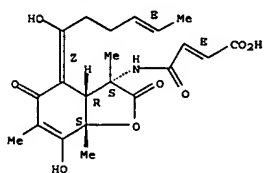
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The saltwater culture of a *P. chrysogenum* strain isolated from the Mediterranean sponge *Ircinia fasciculata* yielded 3 new sorbicillin-derived compounds. whose structures were elucidated mainly by 2D NMR and mass spectrometry. Among them, sorbicillactones A (I) and B (II) are the 1st sorbicillinoid natural products that contain N. I is anti-HIV active and exhibits a strong cytotoxic activity against LS178y leukemic cells, combined with a relatively low toxicity to cervical carcinoma HeLa S3 cells and pheochromocytoma PC 12 cells. The absolute configurations of I and II were elucidated by quantum chemical calcn. of CD spectra. Another compound isolated, sorbivinetone (III), might be an artifact derived from sorbicillinol by Diels-Alder reaction with Et vinyl ether. Furthermore, the known sorbicillinoid fungal metabolites oxosorbicillinol, sorbicillin, and bisvertinolone were identified, as well as the alkaloids melesgrine and roquefortine C. The biosynthetic origin of I from acetate, alanine, and methionine was investigated by feeding expts. with 13C-labeled precursors.

ACCESSION NUMBER: 2005:544137 HCAPLUS
 DOCUMENT NUMBER: 143:244730
 TITLE: The first sorbicillinoid alkaloids, the antileukemic sorbicillactones A and B, from a sponge-derived *Penicillium chrysogenum* strain
 AUTHOR(S): Bringmann, Gerhard; Lang, Gerhard; Gulder, Tobias A. M.; Tsuruta, Hideyuki; Muhlbacher, Jorg; Maksimenka, Katja; Steffens, Stefan; Schaumann, Karsten; Stohr, Ruediger; Wiese, Jutta; Imhoff, Johannes P.; Perovic-Ottstadt, Sanja; Boreiko, Olexandra; Muller, Werner E. G.
 CORPORATE SOURCE: Institut für Organische Chemie, Universität Würzburg, Würzburg, D-97074, Germany
 SOURCE: Tetrahedron (2005), 61(30), 7252-7265
 CODEN: TETRAH; ISSN: 0040-4020
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 861434-14-2P, Sorbicillactone B
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (antileukemic sorbicillinoid alkaloids sorbicillactones A and B from sponge-derived *Penicillium chrysogenum* strain)
 RN 861434-14-2 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[[4E]-1-hydroxy-4-hexenylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuran-2-yl]amino]-4-oxo-, (2E)- (9CI) (CA INDEX NAME)]

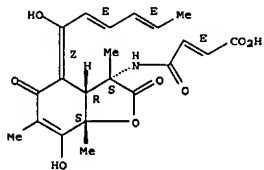
Absolute stereochemistry.
 Double bond geometry as shown.

L4 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)



IT 664987-12-6P, Sorbicillactone A
 RL: BEU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
 (antileukemic sorbicillinoid alkaloids sorbicillactones A and B from sponge-derived *Penicillium chrysogenum* strain)
 RN 664987-12-6 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[(2E,4E)-1-hydroxy-2,4-hexadienylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuranyl]amino]-4-oxo-, (2E)- (9CI) (CA INDEX NAME)

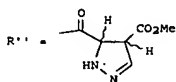
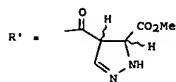
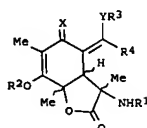
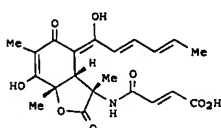
Absolute stereochemistry.
 Double bond geometry as shown.



IT 861434-12-0P
 RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
 (antileukemic sorbicillinoid alkaloids sorbicillactones A and B from sponge-derived *Penicillium chrysogenum* strain)
 RN 861434-12-0 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[(2E,4E)-1-hydroxy-2,4-hexadienylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuranyl]amino]-4-oxo-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2006 ACS ON STN
 ED Entered STN: 11 Mar 2004
 GI



AB The compds. Sorbicillactone A (I), its derivs., e.g., II [R1 = H, (un)branched C1-10-alkyl, C3-10-alkenyl, acyl (e.g., CHO, COMe, COCCl3, fumaryl, maleyl, succinyl; optionally the free CO2H can be CO2Me or other ester), R', R'']; R2 = H, (un)branched C1-10-alkyl, acyl (e.g., CHO, COMe);

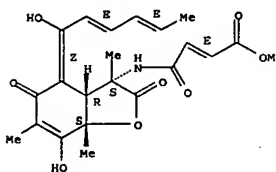
R3 = H, (un)branched C1-10-alkyl, acyl (e.g., CHO, COMe); R4 = (un)branched C1-10-alkyl, C3-10-alkenyl (with 1 or more double bonds); X = O, S, NOH, NOR5; Y = O; XY = N-NH; R5 = (un)branched C1-6-alkyl, their diastereomers, enantiomers and pharmaceutically acceptable salts and solvates, are described, as well as procedures for their production I and II

have antiviral and antitumor characteristics in cell culture models. Further I possesses antiinflammatory characteristics. Finally the biomimetic synthesis of I (or II) is described via oxidative dearomatization of sorbicillin (or its derivative), cyclocondensation with alanine (or another amino acid) and acylation with fumaric acid (or analog).

ACCESSION NUMBER: 2004:198168 HCAPLUS
 DOCUMENT NUMBER: 140:253378
 TITLE: Procedures for the production of Sorbicillactone A and its derivatives and the use of drugs containing them
 INVENTOR(S): Mueller, Werner E. G.; Bringmann, Gerhard; Lang, Gerhard; Muehlbacher, Joerg; Schaumann, Karsten; Steffens, Stefan
 PATENT ASSIGNEE(S): Johannes-Gutenberg-Universitaet Mainz, Germany; Bayerische Julius-Maximilians-Universitaet Wuerzburg
 SOURCE: Ger. Offen., 16 pp.
 CODEN: GWXXBX

Young, Shawquia, Page 6

L4 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)
 Double bond geometry as shown.



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

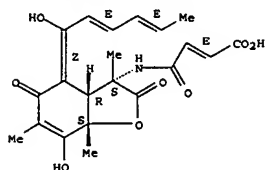
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238257	A1	20040311	DE 2002-10238257	20020821
CA 2496386	AA	20040401	CA 2003-2496386	20030717
WO 2004026854	A1	20040401	WO 2003-EP7805	20030717
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RN:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LJ, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003250985	A1	20040408	AU 2003-250985	20030717
EP 1532129	A1	20050525	EP 2003-797201	20030717
EP 1532129	B1	20061122		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 200603049	T2	20060126	JP 2004-536901	20030717
ZA 2005002226	A	20060222	ZA 2005-2226	20050316
US 2006111420	A1	20060525	US 2005-525685	20050629
PRIORITY APPLN. INFO.:			DE 2002-10238257	A 20020821
			WO 2003-EP7805	M 20030717

OTHER SOURCE(S): CASREACT 140:253378; MARPAT 140:253378

IT 664987-12-6P, Sorbicillactone A
 RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (isolation, reactions, and bioactivity of sorbicillactone A and its derivative)
 RN 664987-12-6 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[(2E,4E)-1-hydroxy-2,4-hexadienylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuranyl]amino]-4-oxo-, (2E)- (9CI) (CA INDEX NAME)

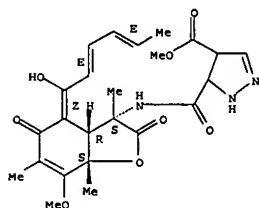
Absolute stereochemistry.
 Double bond geometry as shown.

L4 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 669770-99-4P, SQA-D 1
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (isolation, reactions, and bioactivity of sorbicillactone A and its derivs.)
 RN 669770-99-4 HCAPLUS
 CN 1H-Pyrazole-4-carboxylic acid, 5-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-4-[(2E,4E)-1-hydroxy-2,4-hexadienylidene]-7-methoxy-3,6,7a-trimethyl-2,5-dioxo-3-benzofuranyl]amino]carbonyl]-4,5-dihydro-, methyl ester (9CI) (CA INDEX NAME)

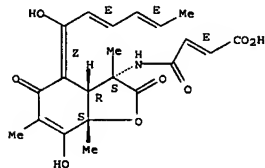
Absolute stereochemistry.
 Double bond geometry as shown.



L4 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

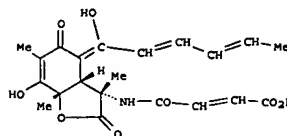
(isolation and characterization of the bioactive alkaloid sorbicillactone A from a sponge-derived fungus)
 RN 664987-12-6 HCAPLUS
 CN 2-Butenoic acid, 4-[[[(3S,3aR,4Z,7aS)-2,3,3a,4,5,7a-hexahydro-7-hydroxy-4-[(2E,4E)-1-hydroxy-2,4-hexadienylidene]-3,6,7a-trimethyl-2,5-dioxo-3-benzofuranyl]amino]-4-oxo-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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 ED Entered STN: 08 Oct 2003
 GI



AB This chapter deals with the discovery of sorbicillactone A (I), as an illustrative example of the fruitful cooperation within BIOTECmarin - its isolation and chemical characterization, and its biol. activities are discussed. I was isolated from a strain of *Penicillium chrysogenum* cultured from a sample of the Mediterranean sponge *Ircinia fasciculata*;

it possesses a unique bicyclic lactone structure, seemingly derived from sorbicillin. Among the numerous known sorbicillin-derived structures, I is the first found to contain nitrogen and thus the first representative of a novel type of sorbicillin alkaloids, apparently originating from a likewise remarkable biosynthesis. Furthermore, I exhibits promising activities in several mammalian and viral test systems, in particular a highly selective cytostatic activity against murine leukemic lymphoblasts (LS178y) and the ability to protect human T cells against the cytopathic effects of HIV-1. These properties qualify sorbicillactone A or one of its derivs. for animal and (hopefully) also future therapeutic human trials.

ACCESSION NUMBER: 2003:786436 HCAPLUS
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 AUTHOR(S): Bringmann, G.; Lang, G.; Muehlbacher, J.; Schaumann, K.; Steffens, S.; Rytik, P. G.; Hentschel, U.; Moraschaeuser, J.; Mueller, W. E. G.
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 IT 664987-12-6P, Sorbicillactone A
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)